

Correction to “The Nature of BH_4^- Reorientations in Hexagonal LiBH_4 ”

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In this paper, we inadvertently presented two different r variables, which may have been confusing to the reader. The r variable in eq 2 is defined as the radius of the circle containing three equidistant H atoms, akin to any three H atoms of the tetrahedral BH_4^- anion. In this case, $r\sqrt{3}$ is the reorientational jump distance between H sites. We initially mention that this r variable is exactly equal to the B–H bond length ($d_{\text{B-H}}$). This is incorrect. This r variable is actually equal to $[(2\sqrt{2})/3]d_{\text{B-H}} \approx 0.94d_{\text{B-H}}$. Further along, in eq 3, we define another variable: $a = (2r)/\sqrt{3}$. The r variable in this equation is indeed equal to $d_{\text{B-H}}$, as is the subsequent r variable in eq 4. In contrast, the r in eqs 5 and 6 and in the Supporting Information refers back to the original r variable in eq 2 and is again equal to $[(2\sqrt{2})/3]d_{\text{B-H}}$. Finally, the earlier statement at the bottom of page 1615 that we used a B–H bond length of 1.14 Å in all of our models is also incorrect. The correct value (which we used) is 1.21 Å. It should be noted that the inconsistent description of r variables and the B–H bond length discussed above have no impact on the validity of the figures, discussion, or scientific conclusions.

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